

1. INTRODUCTION

This volume presents the algorithms used to describe the transport and transformation of chemicals in the TRIM.FaTE module. These algorithms are used to estimate the physical and chemical processes that drive chemical transport and transformation in the environment. As explained in Volume I of this report, the TRIM.FaTE framework can incorporate first-order and higher order algorithms. At the present time, however, only first-order algorithms have been implemented in the model.

First-order transfer between compartments in TRIM.FaTE is described by **transfer factors**, referred to as T-factors. This volume documents all of the T-factors currently implemented in TRIM.FaTE. A T-factor is approximately the instantaneous flux of the chemical in the receiving compartment normalized by the amount of chemical in the sending compartment (see Section 4.2 in Volume I of this report for more discussion about the units of T-factors and related issues). That is, $T * N(t)$ is the instantaneous flux in units of chemical mass/time, where $N(t)$ is the chemical mass in the sending compartment at time t . The compartment that receives the mass lost from the sending compartment is referred to as the receiving compartment.

The **transfer factor**, or T-factor, is the instantaneous chemical flux normalized by the current chemical mass in the sending compartment. That is, T-factors are time-dependent.

Because it is a normalized flux, a large T-factor in itself does not imply that the flux is large; the actual flux also depends on the amount of chemical in the sending compartment. The T-factor is not the same as the fraction of mass lost in a given time interval, although the two quantities are related. When the fraction of mass lost is small, these two quantities are generally approximately the same, but they differ significantly when the fraction of mass lost is larger. In particular, $T = -\ln(1-p)$, where p is the fraction of mass lost in one simulation time step, and the units of time are the same as T.

Chapter 2 presents a general description of how each of the different transport and transformation processes are modeled in TRIM.FaTE. Chapters 3 through 6 present the abiotic algorithms for air (Chapter 3), surface water and sediment (Chapter 4), soil (Chapter 5), and ground water (Chapter 6). For simplicity, the algorithms used to describe intermedia transport are only presented in one of the chapters and referenced in the other.

Chapter 7 presents the algorithms used to describe transport of chemical mass between biotic compartment types and between biotic and abiotic compartment types. Chapters 3 through 7 begin with a brief summary of the algorithms described in the chapter and then explain each algorithm in greater detail. While Chapters 2 through 7 focus on the general algorithms used in TRIM.FaTE, Appendix A presents the chemical-specific algorithms for mercury and PAHs.

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